

^{aka.}
REQUESTED (NARROWER)

Berch 10_688606

09/13/2005

=> file registry

FILE 'REGISTRY' ENTERED AT 10:13:08 ON 13 SEP 2005

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 12 SEP 2005 HIGHEST RN 862971-50-4

DICTIONARY FILE UPDATES: 12 SEP 2005 HIGHEST RN 862971-50-4

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

*
* The CA roles and document type information have been removed from *
* the IDE default display format and the ED field has been added, *
* effective March 20, 2005. A new display format, IDERL, is now *
* available and contains the CA role and document type information. *
*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
<http://www.cas.org/ONLINE/DBSS/registryss.html>

=> file caplus

FILE 'CAPLUS' ENTERED AT 10:13:30 ON 13 SEP 2005

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FILE COVERS 1907 - 13 Sep 2005 VOL 143 ISS 12

FILE LAST UPDATED: 12 Sep 2005 (20050912/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate

(structure
searched
is attached
as
structure "L19")

substance identification.

'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

=> file uspatfull

FILE 'USPATFULL' ENTERED AT 10:13:36 ON 13 SEP 2005

CA INDEXING COPYRIGHT (C) 2005 AMERICAN CHEMICAL SOCIETY (ACS)

FILE COVERS 1971 TO PATENT PUBLICATION DATE: 8 Sep 2005 (20050908/PD)

FILE LAST UPDATED: 8 Sep 2005 (20050908/ED)

HIGHEST GRANTED PATENT NUMBER: US6941576

HIGHEST APPLICATION PUBLICATION NUMBER: US2005198721

CA INDEXING IS CURRENT THROUGH 8 Sep 2005 (20050908/UPCA)

ISSUE CLASS FIELDS (/INCL) CURRENT THROUGH: 8 Sep 2005 (20050908/PD)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2005

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2005

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>>> USPAT2 is now available.  USPATFULL contains full text of the  <<<
>>> original, i.e., the earliest published granted patents or  <<<
>>> applications.  USPAT2 contains full text of the latest US  <<<
>>> publications, starting in 2001, for the inventions covered in  <<<
>>> USPATFULL.  A USPATFULL record contains not only the original  <<<
>>> published document but also a list of any subsequent  <<<
>>> publications.  The publication number, patent kind code, and  <<<
>>> publication date for all the US publications for an invention  <<<
>>> are displayed in the PI (Patent Information) field of USPATFULL  <<<
>>> records and may be searched in standard search fields, e.g., /PN, <<<
>>> /PK, etc.  <<<
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>>> USPATFULL and USPAT2 can be accessed and searched together  <<<
>>> through the new cluster USPATALL.  Type FILE USPATALL to  <<<
>>> enter this cluster.  <<<
>>>  <<<
>>> Use USPATALL when searching terms such as patent assignees,  <<<
>>> classifications, or claims, that may potentially change from  <<<
>>> the earliest to the latest publication.  <<<
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This file contains CAS Registry Numbers for easy and accurate substance identification.

=> file casreact

FILE 'CASREACT' ENTERED AT 10:13:41 ON 13 SEP 2005

USE IS SUBJECT TO THE TERMS OF YOUR CUSTOMER AGREEMENT

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Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE CONTENT:1840 - 11 Sep 2005 VOL 143 ISS 11

New CAS Information Use Policies, enter HELP USAGETERMS for details.

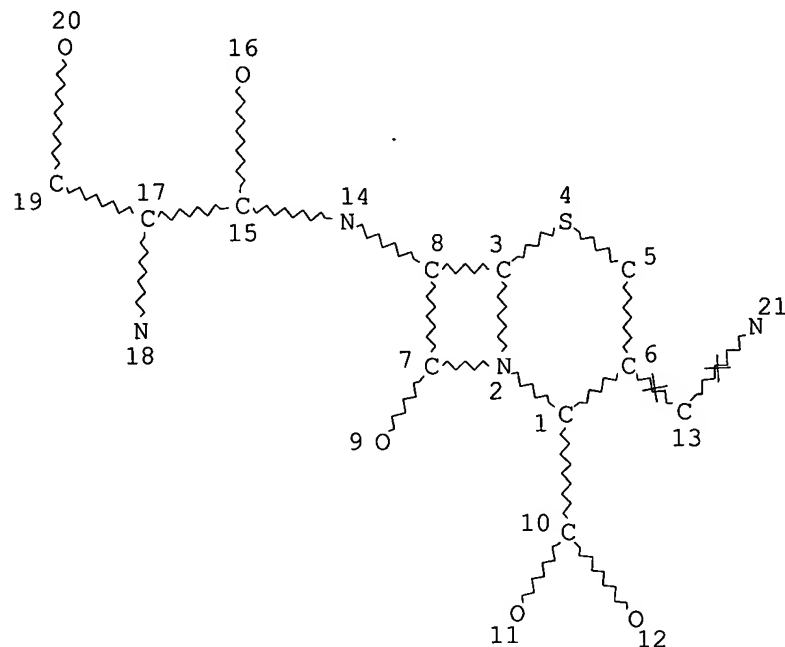
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*****
*
*      CASREACT now has more than 9.2 million reactions      *
*
*****
```

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d stat que L23

L15 STR



NODE ATTRIBUTES:

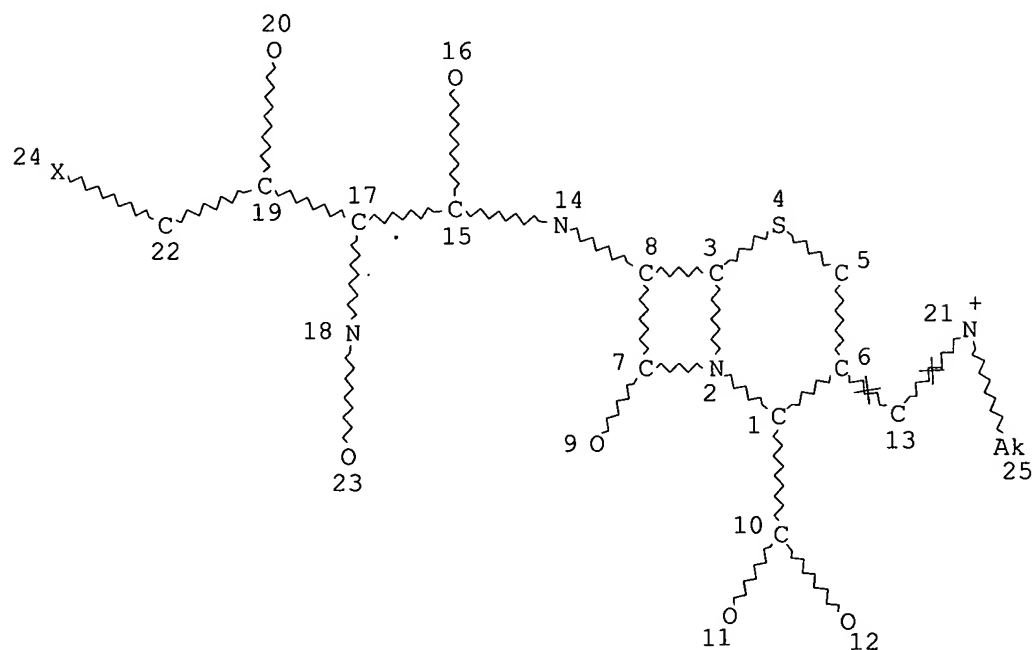
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 CONNECT IS E1 RC AT 20
 DEFAULT MLEVEL IS ATOM
 MLEVEL IS CLASS AT 9 10 11 12 13 14 15 16 17 18 19 20 21
 DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
 RING(S) ARE ISOLATED OR EMBEDDED
 NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

L17 49 SEA FILE=REGISTRY SSS FUL L15
 L19 STR



NODE ATTRIBUTES:

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NSPEC	IS	C	AT	15

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NSPEC   IS C      AT 23
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MLEVEL  IS CLASS AT 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
DEFAULT ECLEVEL IS LIMITED

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GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 25

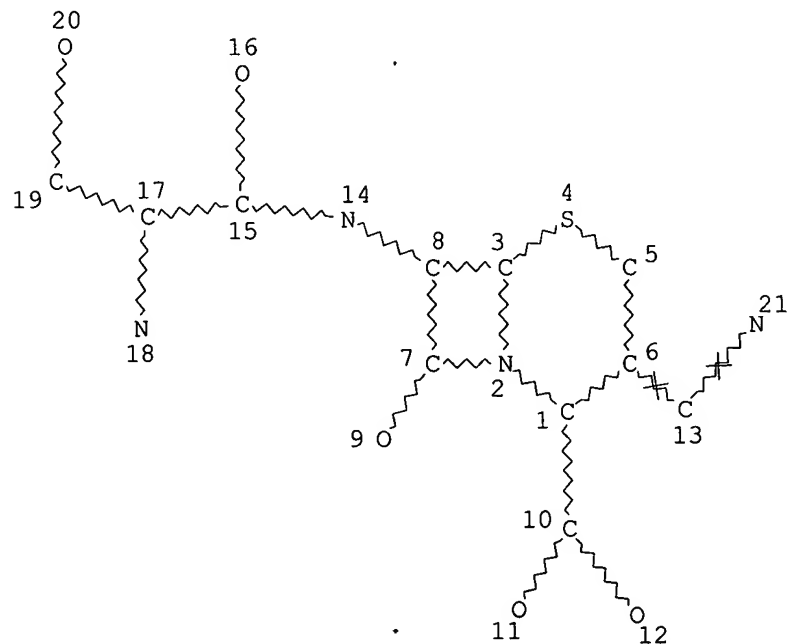
STEREO ATTRIBUTES: NONE

L22 8 SEA FILE=REGISTRY SUB=L17 SSS FUL L19

L23 2 SEA FILE=CAPLUS ABB=ON PLU=ON L22

=> d stat que L28

L15 STR



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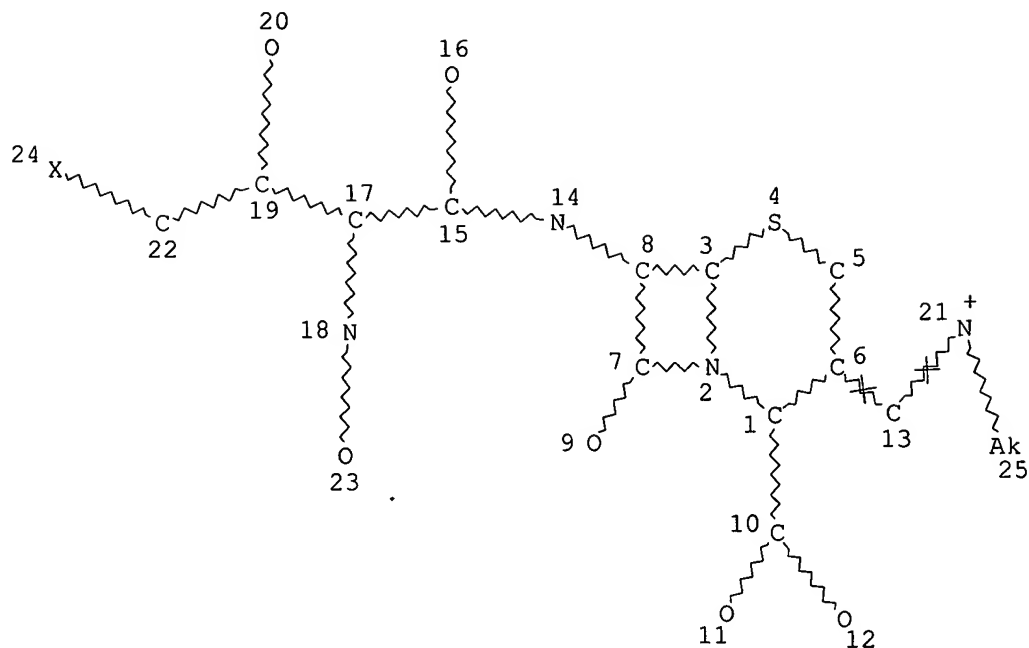
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NSPEC	IS C	AT	16
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CONNECT	IS E1 RC	AT	9
CONNECT	IS E3 RC	AT	10
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CONNECT	IS E3 RC	AT	15
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DEFAULT MLEVEL IS ATOM			
MLEVEL	IS CLASS	AT	9 10 11 12 13 14 15 16 17 18 19 20 21
DEFAULT ECLEVEL IS LIMITED			

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

L17 49 SEA FILE=REGISTRY SSS FUL L15
L19 STR



NODE ATTRIBUTES:

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NSPEC	IS	R	AT	8	
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NSPEC	IS	C	AT	10	
NSPEC	IS	C	AT	11	
NSPEC	IS	C	AT	12	
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CONNECT	IS	E3	RC	AT	17

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 DEFAULT ECLEVEL IS LIMITED

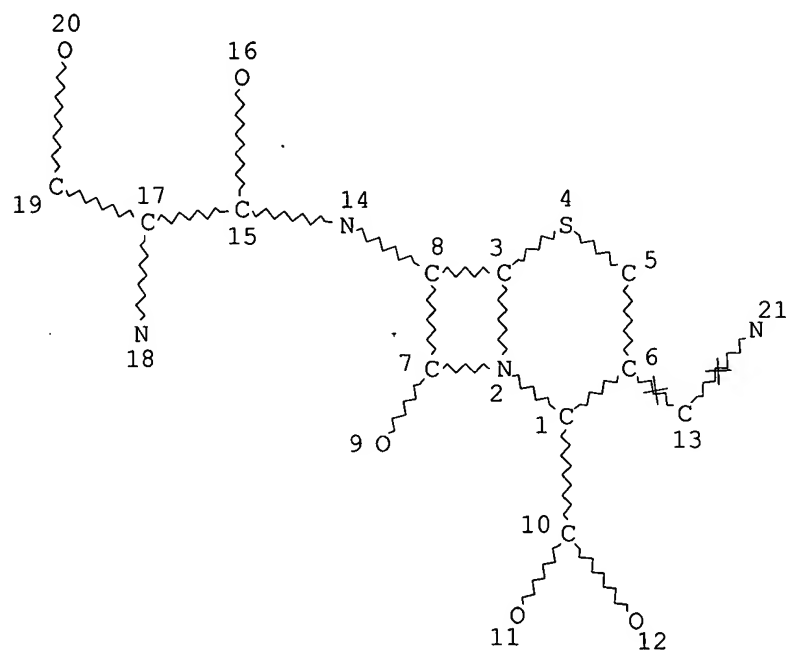
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STEREO ATTRIBUTES: NONE

L22 8 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
 L28 2 SEA L22 *USPATFULL, CASREACT hits*

=> d que L29

L15 STR



NODE ATTRIBUTES:

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NSPEC	IS C	AT	11
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 CONNECT IS E3 RC AT 7
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 DEFAULT ECLEVEL IS LIMITED

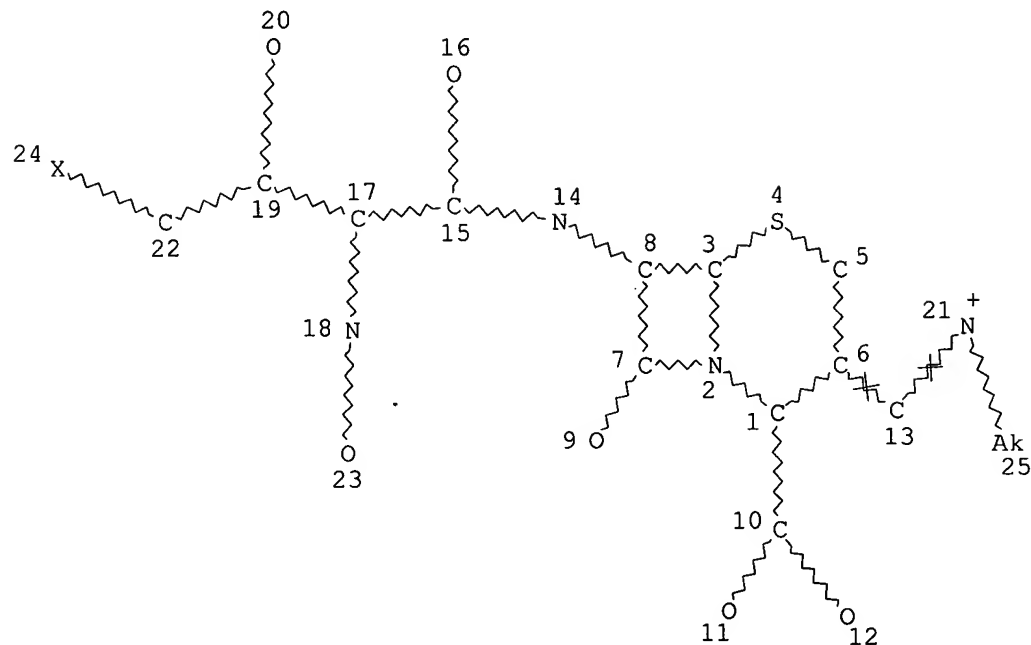
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STEREO ATTRIBUTES: NONE

L17 49 SEA FILE=REGISTRY SSS FUL L15

L19 STR



NODE ATTRIBUTES:

CHARGE IS *+ AT 21
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DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
L22 8 SEA FILE=REGISTRY SUB=L17 SSS FUL L19
L23 2 SEA FILE=CAPLUS ABB=ON PLU=ON L22
L28 2 SEA L22
L29 2 DUP REM L23 L28 (2 DUPLICATES REMOVED)

=> file stnguide
FILE 'STNGUIDE' ENTERED AT 10:15:04 ON 13 SEP 2005
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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.
LAST RELOADED: Sep 9, 2005 (20050909/UP).

=> d ibib abs hitstr L29 1-2
YOU HAVE REQUESTED DATA FROM FILE 'CAPLUS' - CONTINUE? (Y)/N:y

L29 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2005:160883 CAPLUS
DOCUMENT NUMBER: 142:261334

TITLE: Process for preparing cefepime by the
cyclocondensation reaction of thiourea with a
brominated or chlorinated derivative

INVENTOR(S): Handa, Vijay Kumar; Kamat, Anand G.; Sivakumaran,
Meenakshisunderam

PATENT ASSIGNEE(S): India

SOURCE: U.S. Pat. Appl. Publ., 5 pp.
CODEN: USXXCO

DOCUMENT TYPE: Patent

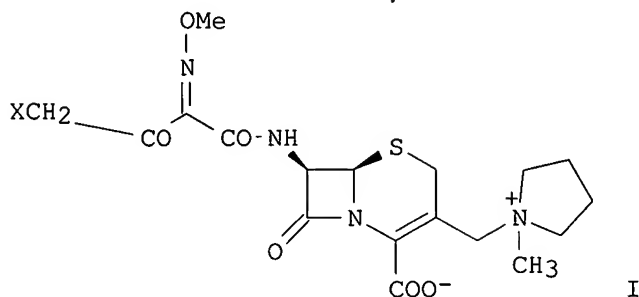
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2005043531	A1	20050224	US 2003-688606	20031017
PRIORITY APPLN. INFO.:			IN 2003-CH669	A 20030821
OTHER SOURCE(S):		CASREACT 142:261334		

GI



AB Cefepime, a cephalosporin antibiotic, is prepared in high yield and selectivity by the cyclocondensation of thiourea with bromo or chloro derivative I (X = Br, Cl) which is prepared by the amidation of 7-amino-3-[(1-methyl-1-pyrrolidinium)methyl]-3-cephem-4-carboxylate with a corresponding 4-halo-2-methoxyimino-3-oxobutyric acid halide. Thus, cefepime dihydrochloride monohydrate was prepared from 7-amino-3-[(1-methyl-1-pyrrolidinium)methyl]-3-cephem-4-carboxylate hydrochloride via silylation with Me₃SiNHAc in CH₂Cl₂, acylation with freshly prepared 4-bromo-2-methoxyimino-3-oxobutyl chloride in CH₂Cl₂ and cyclocondensation of intermediate I (X = Br) with H₂NC(:S)NH₂ in aqueous MeCOMe.

IT 846021-46-3P 846021-47-4P 846021-48-5P

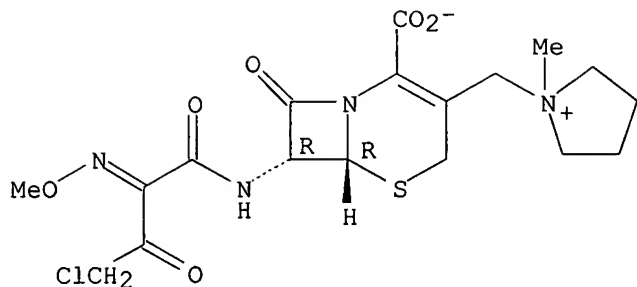
RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(in a process for preparing cefepime by the cyclocondensation reaction of thiourea with a brominated or chlorinated derivative)

RN 846021-46-3 CAPLUS

CN Pyrrolidinium, 1-[[[(6R,7R)-2-carboxy-7-[[4-chloro-2-(methoxyimino)-1,3-dioxobutyl]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-methyl-, inner salt (9CI) (CA INDEX NAME)

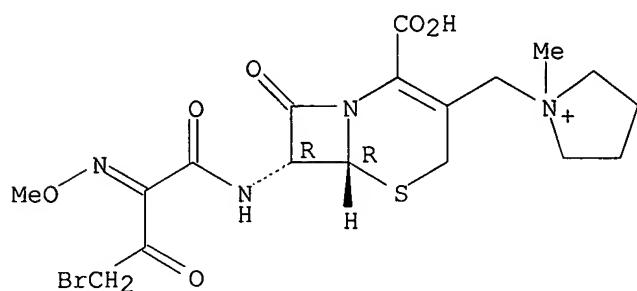
Absolute stereochemistry.
Double bond geometry unknown.



RN 846021-47-4 CAPLUS.

CN Pyrrolidinium, 1-[[(6R, 7R)-7-[[4-bromo-2-(methoxyimino)-1,3-dioxobutyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.

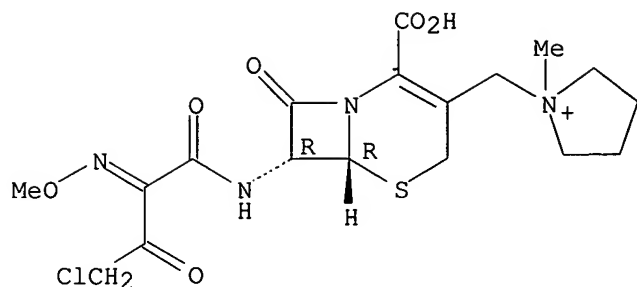


● Cl⁻

RN 846021-48-5 CAPLUS

CN Pyrrolidinium, 1-[[(6R, 7R)-2-carboxy-7-[[4-chloro-2-(methoxyimino)-1,3-dioxobutyl]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry unknown.



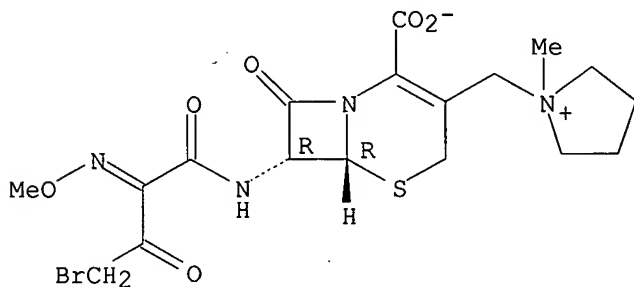
IT 846021-45-2P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (process for preparing cefepime by the cyclocondensation reaction of thiourea with a brominated or chlorinated derivative)

RN 846021-45-2 CAPLUS

CN Pyrrolidinium, 1-[[[(6R,7R)-7-[[4-bromo-2-(methoxyimino)-1,3-dioxobutyl]amino]-2-carboxy-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-methyl-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



L29 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:902392 CAPLUS

DOCUMENT NUMBER: 141:366239

TITLE: A preparation of antibacterial 5-thia-1-azabicyclo[4.2.0]octane derivative (cefepime)
 INVENTOR(S): Ludescher, Johannes; Sturm, Hubert; Wolf, Siegfried
 PATENT ASSIGNEE(S): Sandoz A.-G., Switz.
 SOURCE: PCT Int. Appl., 28 pp.
 CODEN: PIXXD2

DOCUMENT TYPE: Patent
 LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2004092183 A2 20041028 WO 2004-EP3988 20040415
 WO 2004092183 A3 20041209
 W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH,
 CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
 GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
 LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
 NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
 TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,
 BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE,
 ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI,
 SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN,
 TD, TG

PRIORITY APPLN. INFO.:

AT 2003-584

A 20030416

AT 2003-585

A 20030416

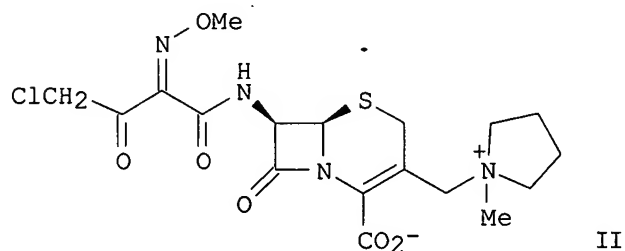
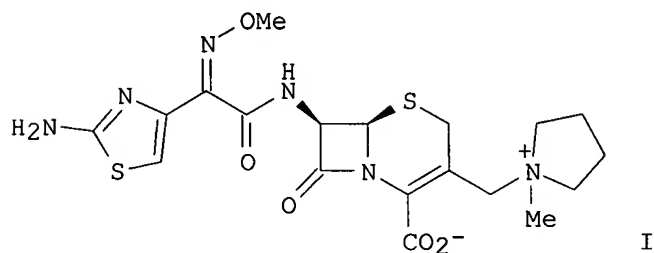
AT 2003-586

A 20030416

OTHER SOURCE(S):

MARPAT 141:366239

GI



AB The invention relates to a preparation of 5-thia-1-azabicyclo[4.2.0]octane derivative I (cefepime), useful as antibacterial agent (no biol. data). For instance, 5-thia-1-azabicyclo[4.2.0]octane derivative (I•2HCl) was prepared via heterocyclization of chloro(methoxyimino)oxobutyric acid derivative II•HCl and thiourea (example 3, 99.6% of purity).

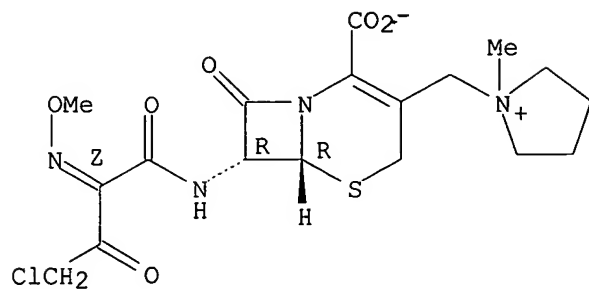
IT **780810-16-4P 780810-18-6P**

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of antibacterial cefepime from thiaazabicyclo[4.2.0]octane derivs. and thiourea)

RN 780810-16-4 CAPLUS-

CN Pyrrolidinium, 1-[[[(6R,7R)-2-carboxy-7-[[[(2Z)-4-chloro-2-(methoxyimino)-1,3-dioxobutyl]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-methyl-, inner salt, monohydrochloride (9CI) (CA INDEX NAME)

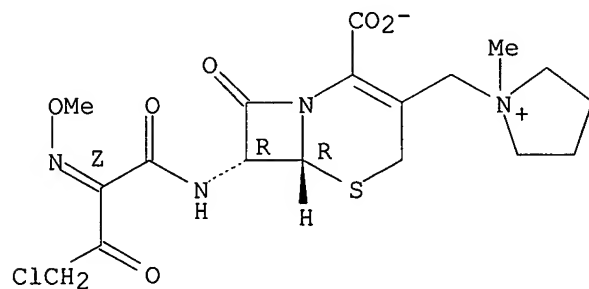
Absolute stereochemistry.
Double bond geometry as shown.



● HCl

RN 780810-18-6 CAPLUS
CN Pyrrolidinium, 1-[[(6R,7R)-2-carboxy-7-[[(2Z)-4-chloro-2-(methoxyimino)-1,3-dioxobutyl]amino]-8-oxo-5-thia-1-azabicyclo[4.2.0]oct-2-en-3-yl]methyl]-1-methyl-, inner salt (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



Beilstein search on narrower (requested) structure

Berch 10_688606

09/13/2005

=> file beilstein

FILE 'BEILSTEIN' ENTERED AT 10:23:30 ON 13 SEP 2005

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= no hits

FILE RELOADED ON OCTOBER 20, 2002

FILE LAST UPDATED ON JUNE 29, 2005

FILE COVERS 1771 TO 2005.

*** FILE CONTAINS 9,271,550 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in separate documents and can not be searched together in one query. Reaction data for BEILSTEIN compounds may be displayed immediately with the display codes PRE (preparations) and REA (reactions). A substance answer set retrieved after the search for a chemical name, a compounds with available reaction information by combining with PRE/FA, REA/FA or more generally with RX/FA. The BEILSTEIN Registry Number (BRN) is the link between a BEILSTEIN compound and belonging reactions. For more detailed reaction searches BRNs can be searched as reaction partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

>>> FOR SEARCHING PREPARATIONS SEE HELP PRE <<<

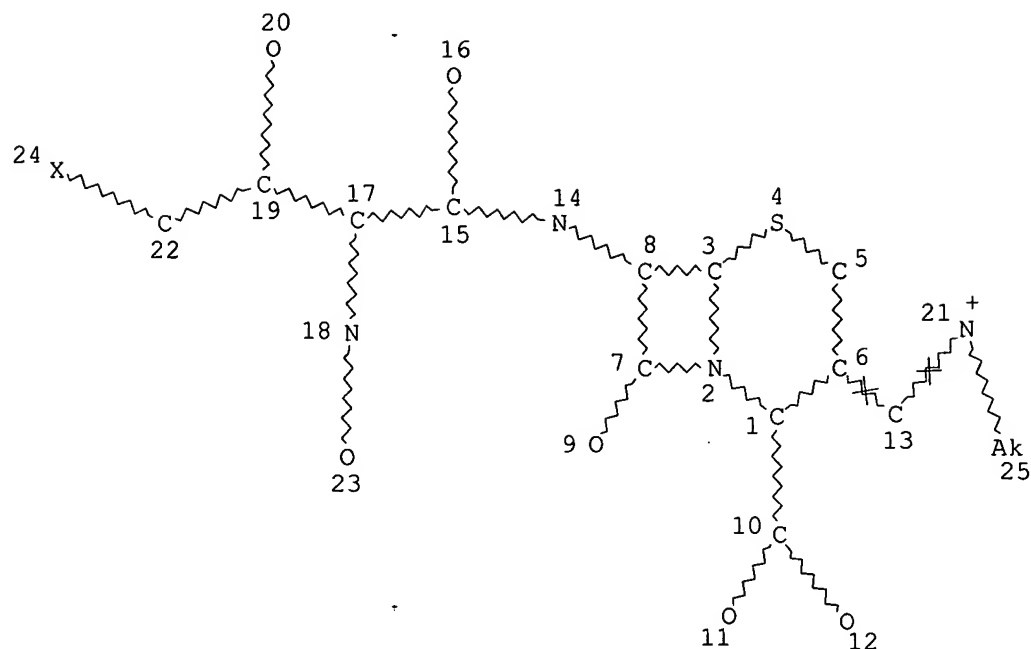
* PLEASE NOTE THAT THERE ARE NO FORMATS FREE OF COST. *
* SET NOTICE FEATURE: THE COST ESTIMATES CALCULATED FOR SET NOTICE *
* ARE BASED ON THE HIGHEST PRICE CATEGORY. THEREFORE; THESE *
* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS. *
* FOR PRICE INFORMATION SEE HELP COST *

NEW

* PATENT NUMBERS (PN) AND BABS ACCESSION NUMBERS (BABSAN) CAN NOW BE SEARCHED, SELECTED AND TRANSFERRED.
* NEW DISPLAY FORMATS ALLREF, ALLP AND BABSAN SHOW ALL REFERENCES, ALL PATENT REFERENCES, OR ALL BABS ACCESSION NUMBERS FOR A COMPOUND AT A GLANCE.

=> d stat que L30

L19 STR



NODE ATTRIBUTES:

CHARGE	IS	++	AT	21	
NSPEC	IS	R	AT	1	
NSPEC	IS	R	AT	2	
NSPEC	IS	R	AT	3	
NSPEC	IS	R	AT	4	
NSPEC	IS	R	AT	5	
NSPEC	IS	RC	AT	6	
NSPEC	IS	R	AT	7	
NSPEC	IS	R	AT	8	
NSPEC	IS	C	AT	9	
NSPEC	IS	C	AT	10	
NSPEC	IS	C	AT	11	
NSPEC	IS	C	AT	12	
NSPEC	IS	RC	AT	13	
NSPEC	IS	C	AT	14	
NSPEC	IS	C	AT	15	
NSPEC	IS	C	AT	16	
NSPEC	IS	C	AT	17	
NSPEC	IS	C	AT	18	
NSPEC	IS	C	AT	19	
NSPEC	IS	C	AT	20	
NSPEC	IS	RC	AT	21	
NSPEC	IS	C	AT	22	
NSPEC	IS	C	AT	23	
NSPEC	IS	C	AT	24	
NSPEC	IS	C	AT	25	
CONNECT	IS	E3	RC	AT	7
CONNECT	IS	E1	RC	AT	9
CONNECT	IS	E3	RC	AT	10
CONNECT	IS	E1	RC	AT	11
CONNECT	IS	E3	RC	AT	15
CONNECT	IS	E1	RC	AT	16
CONNECT	IS	E3	RC	AT	17

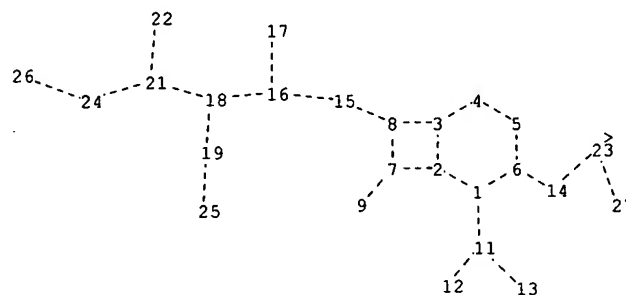
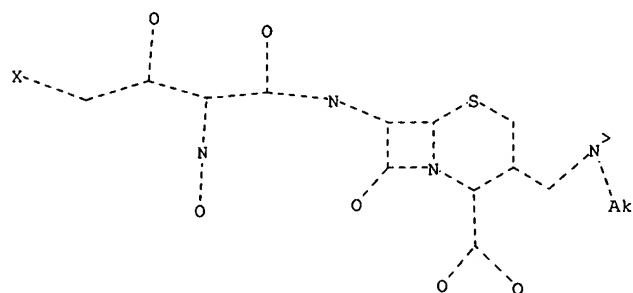
CONNECT IS E3 RC AT 19
CONNECT IS E1 RC AT 20
DEFAULT MLEVEL IS ATOM
MLEVEL IS CLASS AT 9 10 11 12 13 14 15 16 17 18 19 20 21 22 23 24 25
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 25

STEREO ATTRIBUTES: NONE
L30 0 SEA FILE=BEILSTEIN SSS FUL L19

100.0% PROCESSED 84 ITERATIONS
SEARCH TIME: 00.00.04

0 ANSWERS



chain nodes :

9 11 12 13 15 16 17 18 19 21 22 24 25 26 27

ring nodes :

1 2 3 4 5 6 7 8

ring/chain nodes :

14 23

chain bonds :

1-11 7-9 8-15 11-12 11-13 15-16 16-17 16-18 18-19 18-21 19-25 21-22 21-24
23-27 24-26

ring/chain bonds :

6-14 14-23

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-8 4-5 5-6 7-8

exact/norm bonds :

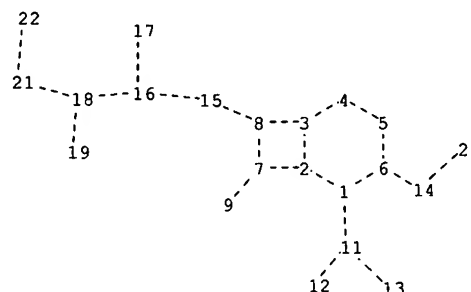
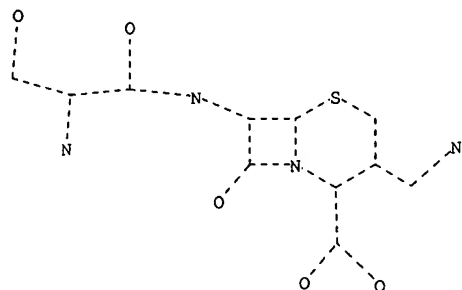
1-2 1-6 1-11 2-3 2-7 3-4 3-8 4-5 5-6 6-14 7-8 7-9 8-15 11-12 11-13 14-23
15-16 16-17 16-18 18-19 18-21 19-25 21-22 21-24 23-27 24-26

Connectivity :

7:3 E exact RC ring/chain 9:1 E exact RC ring/chain 11:3 E exact RC ring/chain
12:1 E exact RC ring/chain 16:3 E exact RC ring/chain 17:1 E exact RC ring/chain
18:3 E exact RC ring/chain 21:3 E exact RC ring/chain 22:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS
22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS



chain nodes :

9 11 12 13 15 16 17 18 19 21 22

ring nodes :

1 2 3 4 5 6 7 8

ring/chain nodes :

14 23

chain bonds :

1-11 7-9 8-15 11-12 11-13 15-16 16-17 16-18 18-19 18-21 21-22

ring/chain bonds :

6-14 14-23

ring bonds :

1-2 1-6 2-3 2-7 3-4 3-8 4-5 5-6 7-8

exact/norm bonds :

1-2 1-6 1-11 2-3 2-7 3-4 3-8 4-5 5-6 6-14 7-8 7-9 8-15 11-12 11-13 14-23
15-16 16-17 16-18 18-19 18-21 21-22

Connectivity :

7:3 E exact RC ring/chain 9:1 E exact RC ring/chain 11:3 E exact RC ring/chain
12:1 E exact RC ring/chain 16:3 E exact RC ring/chain 17:1 E exact RC ring/chain
18:3 E exact RC ring/chain 21:3 E exact RC ring/chain 22:1 E exact RC ring/chain

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:CLASS 11:CLASS
12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS 21:CLASS
22:CLASS 23:CLASS